

2-Methylheptane
592-27-8 | DTXSID2060460

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $8.88\text{e-}12\text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $8.68\text{e-}01$

Confidence level: $9.07\text{e-}01$

Nearest Neighbors from the Training Set

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Nonane

Measured: $1.02\text{e-}11$

Predicted: $8.45\text{e-}12$

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Decane

Measured: $1.16\text{e-}11$

Predicted: $1.10\text{e-}11$

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Hexane, 2,2-dimethyl-

Measured: $4.83\text{e-}12$

Predicted: $5.67\text{e-}12$

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2-Methyloctane

Measured: $1.01\text{e-}11$

Predicted: $9.18\text{e-}12$

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4-Methyloctane

Measured: $9.72\text{e-}12$

Predicted: $9.18\text{e-}12$